FINAL PERFORMANCE REPORT
GRANT No. DE-FG02-96ER25301

RECEIVED
APR 17 2000
OSTI

HAMPTON UNIVERSITY UNDERGRADUATE COMPUTATIONAL
SCIENCE EDUCATION PROGRAM

SUMMARY

The achievements in the two and a half years of this project completely satisfy and exceed the goals and objectives established in the original proposal. The educational tasks have been performed, and its objectives have been satisfied and surpassed. Furthermore, with an efficient allocation of the funding provided by the Grant supplemented by additional University funds, we have established a sustainable infrastructure that provides access to the prevalent paradigms of high performance computation, and is the foundation for future access to distributed parallel computation. This access is extended beyond Hampton University through cooperation and support to regional institutions, in particular to researchers from DOE's Jefferson Lab in Newport News, Virginia.

The resources, deployed in a specially prepared location provided by the School of Science, include a parallel distributed shared memory Silicon Graphics Origin 2000 and a traditional shared memory parallel vector processor Cray EL98. A strategic objective of the Grant was to increase and enhance the participation of under represented minorities in computational science and simulation. These resources and cooperation help create the environment and opportunities, rarely available in Minority Institutions, for faculty and students to enhance or develop expertise in the latest computational technologies and use them in their disciplines.

We have no objection from a patent standpoint to the publication or dissemination of this material.

MPDvorsak
Office of Intellectual
Property Counsel
DOE Field Office, Chicago

4-12-00
Date

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

DETAILED PERFORMANCE

Since August 15, 1996, the starting date of the Grant, until February 14, 1999, the ending date of the Grant (after a six months no-cost extension), the following activities related with the objectives of the grant were conducted by the Principal Investigator Dr. E. A. Socolovsky:

- Preparation and teaching of the 1997 and 1998 summer computational science courses in coordination with Dr. Edward Hill (formerly at DOE) from the SEMS Scholarship program, as stated in the grant proposal.
- Configuration and acquisition of the equipment funded in the first year budget :
 - Close cooperation with the representative of Silicon Graphics / Cray in configuring the equipment and other areas, has facilitated obtaining free upgrades to a more powerful and expandable CRAY EL-98, and larger memories.
 - Purchased an SGI High Impact workstation with video capabilities, e.g., to produce tapes of animations of computations and video conferencing.
- Selection, configuration and acquisition of equipment reassigning equipment funds for the second year, supplemented by other University funds:
 - Close cooperation with the representative of Silicon Graphics allowed us to purchase an **Origin 2000** with 8 processors and 512 MB of memory and 13.5 GB of disk storage, and to participate in SGI's **Varsity (software) Program**, both at a specially discounted price.

- Coordination and supervision of site preparation (230V power, A/C, 100 Mbits ethernet), including the purchase and assembly of a high performance Matrix 5000 Uninterruptible Power Source (UPS), to protect the equipment from black-, brown-outs, and other power problems.
 - Two Jazz SCSI drives for portable 1 GB and 2 GB disk cartridges, to facilitate back-up and use of user files.
 - Purchase and installation of upgrades for the High Impact workstation: 64 MB memory expansion, 12X CD-ROM and US Robotics Courier V Everything Modem.
-
- Supervision of Graduate Students totally or partially supported by the Grant: Craig Hanley (9/97 to 12/98) and Mosiane Lotlamoreng (12/98 to 2/99).
 - Screened, selected, hired and presently supervise four undergraduate and one graduate student with different backgrounds, to help prepare materials to be used in the 1997 summer computational science courses and act as teaching assistants. The activities in which these students are involved include:
 - Installation of the CSEP electronic book at Hampton University. This computational science teaching tool will be used in regular courses as well.
 - Joined Dr. Socolovsky at a Cray Fortran 90 workshop at NASA Langley, and prepared help materials to facilitate its use on the EL-98.
 - Installation of graphics software on the SGI and Linux on PC's.
 - Coordination with the Computer Science departments of Hampton and The College of William and Mary which resulted in a joint proposal to the National Science Foundation CISE Educational Innovation Program entitled "Undergraduate Modeling, Simulation and Analysis" which has been funded. Dr. Socolovsky is the PI for Hampton University.

- Participated in the following meetings:
 - Supercomputing '96, Pittsburgh, PA.
 - Supercomputing '97 (SC'97), San Jose, CA.
 - Supercomputing '98 (SC'98), Orlando, FL.
 - DOD/HBCU and MI meeting, Phoenix, AZ.
 - Second SIAM Conf. on Mathematical and Computational Aspects of Materials Science, Philadelphia PA.
 - Interface '98, 29th symposium on the Interface of Computing Science and Statistics
- Convened with members of Jefferson Labs, NASA Langley, Newport News Shipyard, The College of William and Mary, Silicon Graphics and other educational and research institutions, to share resources and cooperate in the area of supercomputing.
- Assisted the Vice President for research in preparing drafts of a position paper on the adoption of high performance computation, communications and visualization as a theme in Hampton's strategic plan. This includes the configuration of a high performance computation, communications and visualization sustainable facility, and the possible establishment of a Ph.D. program in Computational and Applied Science and Mathematics. The seed for this facility is the equipment acquired under this grant, and it will be organized under a service, consulting support and research structure that would serve as a regional resource.
- System management and maintenance.

ACCESS AND COLLABORATION

The following is a list of users from outside of Hampton University, with which we have collaborated in different degrees and provided access and support to use our resources. We have adjoined copy of some of the communications exchanged which provide a brief description of the subject of the computations and people involved.

- Robert T. Siegel, W. F. C. Ferguson Professor of Physics at The College of William and Mary, and collaborators from the University of Moscow, on muonic interactions and bound and resonant states of hydrogen isotope muonic ions.
- Drs. C. Coriano, J. Goity, L. Gordon, R. Lewis and C. Savkli from TJNAF (DOE) and The College of William and Mary, on Lattice Quantum Chromodynamics computations to study hybrid mesons and baryons.
- Dr. Mikhail Gilinsky and his collaborators at NASA Langley and Hampton, on computational studies on noise and drag/thrust benefits using unconventional geometries and materials.
- Dr. Winston Roberts and his collaborators at TJNAF and Old Dominion University, on high energy particle computations like double pion photoproduction.

Expansion Bases in Nuclear Physics

Shannon T. Cowell
Old Dominion University
shannon@physics.odu.edu

January 11, 1999

Mentor: Dr. Winston Roberts
Old Dominion University

Abstract

The harmonic oscillator basis is one that is commonly used for the expansion of the wave functions of systems of particles in hadronic physics. Analytically, many integrals involving these wave functions are easily calculated. Computationally, the gaussian factor provides rapid convergence for all but the most pathological of integrals. These are perhaps the main reasons for the popularity of this basis. However, it is not clear that this basis is the most appropriate for use in solving some of the problems to which it has been applied. It was the intent of this project to determine the appropriateness of this basis in these complex Hamiltonian systems and to pursue the possibility of a more appropriate basis. A comparison was completed between the harmonic oscillator basis and a hydrogen-like Laguerre basis (referred to as the Keister basis). Simple, well-known systems are studied using both bases, and the resulting eigen-energies and wave functions are compared. This comparison is continued through increasingly more detailed and involved Hamiltonians. Preliminary results suggest that, though it may not be the best solution, the Keister basis may be a more suitable expansion basis for treating many of these systems.

Kinetic Energy	Potential	Energy HO Basis	Energy Keister Basis	Expected/ Energy
Non-Relativistic	C	-0.0519755	-0.051984	-0.051984
	C + Sm (S=0)	-0.102112	-0.102124	
	C + Sm (S=1)	-0.0451982	-0.0452046	
	HO	1.43248	1.43248	1.43248
	HO + Sm (S=0)	1.23284	1.2384	
	HO + Sm (S=1)	1.4966	1.4966	
	CL	0.509034	0.509032	
	CL + Sm (S=0)	0.344165	0.344162	
	CL + Sm (S=1)	0.55539	0.555388	
Semi-Relativistic	C	1.94506	1.94498	1.9450 [5]
	C + Sm (S=0)	1.87083	1.87061	
	C + Sm (S=1)	1.95352	1.95347	
	HO	3.28124	3.28124	
	HO + Sm (S=0)	3.05396	3.05396	
	HO + Sm (S=1)	3.3537	3.3537	
	CL	2.45359	2.45347	
	CL + Sm (S=0)	2.24134	2.24116	
	CL + Sm (S=1)	2.51155	2.51145	

Table 2: Energy values obtained for each Hamiltonian considered using 60 basis wave functions. Parameter values are provided in Table 1. The form of each Hamiltonian can be obtained from equations (15)-(20). C = Coulomb, HO = Harmonic Oscillator, CL = Coulomb + Linear, Sm = Smear, S = Total Spin

is our intent to continue this comparison into physical calculations such as decays and form factors of hadrons.

7 Acknowledgements

This project was funded by the National Science Foundation's Research Experience for Undergraduates Program. Many thanks go to Dr. Winston Roberts for his guidance and patience and to Dr. Eduardo Socolovsky for the use of computational equipment.

References

- [1] B. D. Keister and W. N. Polyzou, J. Comp. Phys. **137**, 231 (1997).

Research Project in Lattice Quantum Chromodynamics

This project is concerned with the study of the so called hybrid mesons and baryons by using lattice Quantum Chromodynamics (QCD), and it is expected to be of great relevance for the further understanding of the structure of sub-nuclear constituents. The production of such hybrid hadrons will be investigated in experiments to be conducted using the electron accelerator at the Department of Energy (DOE) Thomas Jefferson Accelerator Facility (TJNAF) in nearby Newport News, VA.

There is a need to provide theoretical predictions for the masses of these hybrids and their decay widths (lifetimes), and the first objective is to provide predictions for the masses of the hybrid mesons, and also to study the use of so called improved actions in lattice gauge field theory. These studies require the use of lattice formulations of the fundamental theory of the strong interactions, QCD. In the proposed computational approach space-time is discretized and the quantum dynamics are then simulated using appropriate Monte Carlo algorithms.

Hybrid correlators on lattices of size $18 \times 18 \times 18 \times 18$ or larger, will be simulated by generating large numbers of gauge field configurations which are stored, and at a later stage retrieved to calculate other elements of the simulation, for instance the quark propagators. Given the lattice size and the number of different hybrid correlators we plan to study, the resulting computations are large scale.

Since the computational method is inherently parallel, with support from Dr. Eduardo Socolovsky, we shall develop scalable parallel code using OpenMP primitives, to exploit the capabilities of the Silicon Graphics Origin 2000 available through the Undergraduate Computational Science Program at Hampton University which is supported by DOE.

The spokespersons for this project are Dr. Claudio Coriano from TJNAF, and Dr. Jose L. Goity from TJNAF and the Physics Department of Hampton University. Other members of the group are Dr. Lionel Gordon from TJNAF, Dr. Randy Lewis from University of Regina (Canada) and currently visiting TJNAF, and Dr. Cetin Savkli from the College of William and Mary.

Subject:

Date: Thu, 21 Jan 1999 22:34:46 GMT

From: Mikhail Gilinsky <gilinsky@ellag.larc.nasa.gov>

DR. Mikhail Gilinsky
Research Professor
Hampton University

**MIXING, NOISE AND DRAG/THRUST BENEFITS
USING UNTRADITIONAL DESIGNS AND/OR PARTICLE INJECTION**

SUMMARY

The Fluid Mechanics Laboratory was established at the Hampton University Engineering and Technology School in June of 1996. The initiation of this laboratory was made possible by a NASA grant NAG-1-1835 (3 year FAR Award, 1996-99) and is supported by a NASA FY 1997 Partnership Award (1997-99), NAG-1-1936. In addition, FML in cooperation with NASA Langley research Center (LaRC) jointly conducts research with the Central AeroHydrodynamics Institute (TsAGI, Moscow) in Russia under a 2 year Civilian Research and Development Foundation (CRDF) grant #RE2-136 (1996-98).

The FML at HU continues to investigate novel and promising concepts for reduction of noise and improvement in efficiency for jet exhaust nozzles and fans, drag reduction of different aircraft elements using permeable surfaces and particle injection into boundary layers or jet flows.

The first concept includes several innovative corrugated nozzle designs, which provide jet noise and thrust benefits for aircraft engine nozzle: A Bluebell, Chisel, Telescope nozzles, Corrugated Separate Flow Co-Annular Nozzle, A Nozzle with the Screwdriver Centerbody (Plug). The current research has focus on further development of these nozzle concept through numerical and experimental simulations. The Bluebell nozzle concept, for which a patent application has been filed through NASA, can be utilized as a noise reduction concept for separate flow co-annular nozzle in the NASA AST program. Already Boeing, GE Aircraft Engines and Pratt & Whitney Aircraft have expressed interest in the development of this concept for subsonic commercial engine technology pending a successful outcome of testing and analysis. The application of this research to the future supersonic US aircraft engine design are also very promising on the base of the preliminary positive results of the experimental and numerical simulations.

The second, a μ -strip concept is intended for improving the working efficiency of propellers and screws. Under this grant

the theoretical analysis and numerical simulation of several different M-shaped designs for air and water flows will be conducted for the purpose of determining the optimal parameters that provide maximum thrust, lift, mixing, and minimal noise. In this research, fabrication of small scale screw models and experimental tests were conducted on available equipment. These and future tests involve cooling, boat propellers, mixing in appliance, blenders, helicopters.

The third, particle injection for jet noise reduction or engine inlet drag reduction. This concept includes creation of new mathematical models for mass-, momentum- and heat- transfer between hot air and water particles in supersonic flow with taking into account multiple physico-chemical processes and mutual interaction. Analysis and modernization of theoretical approaches for correct description of sound propagation in water-air systems. Numerical simulation using the discrete-trajectory approach and NASA CFL3D code based on Navier-Stokes solver.

In general, the goal of current research using HU computer system, including the powerful computer of HU Department of Mathematics, is following: to create of prediction theoretical models, numerical simulation, comparison of theoretical with experimental results, modification of theoretical approaches, models, grids etc. for several complicated 2D and 3D nozzle designs using NASA and own codes based on full and marching Euler and Navier-Stokes solvers: CFL3D, CRAFT, Godunov and others.